

Abstract Submitted
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SrTiO₃ on silicon: interface chemistry, polarization pinning, and electronic states SOHRAB ISMAIL-BEIGI, Yale University, ALEXIE KOLPAK, Massachusetts Institute of Technology, FRED WALKER, JIM REINER, CHARLES AHN, Yale University — We use SrTiO₃/Si as a model system to examine the effects of interface atomic structure and composition on the functional properties of epitaxial oxide films on silicon. Using first-principles computations, we show that intrinsic chemo-mechanical boundary conditions at the interface fix a single polarization direction in the SrTiO₃ thin film independent of the interface composition, inhibiting ferroelectric functionality. In contrast, the transport properties of the interface are quite sensitive to the interface composition, which can be used to tune the interface from an insulator to an interfacial 2D electron gas. We describe the origins of both functionalities and discuss their applicability to the general class of epitaxial oxides on semiconductors.

Alexie Kolpak
Massachusetts Institute of Technology

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